

Low-lying magnon excitations in integer-spin ladders and tubes

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Abstract

We consider low-energy excitation structures of N -leg integer-spin ladder and tube systems with an antiferromagnetic (AF) intrachain coupling and a uniform external field. The tube means the ladder with the periodic boundary condition along the interchain (rung) direction. Odd-leg AF-rung tubes have the frustration. In order to analyze all systems including frustrated tubes, we apply a field-theoretical method based on the nonlinear sigma model. We mainly focus on the systems without any external fields. In this case, it is shown that the lowest bands of frustrated tubes always consist of six-fold degenerate magnon excitations, while those of all other systems are triply degenerate. This result implies that the ground states of frustrated tubes (all non-frustrated systems) become a two (one)-component Tomonaga-Luttinger liquid, when a sufficiently strong uniform field is applied.

Key words: spin ladder, spin tube, frustration, nonlinear sigma model, Tomonaga-Luttinger liquid

1. Introduction

Quasi-one-dimensional (1D) spin systems have attracted much interest theoretically and experimentally for a long time. Recently, spin ladders [1], finite-number coupled spin chains [see Fig. 1(a)], have been studied intensively. In spin ladders with antiferromagnetic (AF) intrachain coupling, it is widely believed that odd-leg and half-integer-spin ladders have a gapless excitation, while other ladders possess a spin gap. A main theoretical support of this prediction is given by the nonlinear sigma model (NLSM) method [2,3,4]. Moreover, it is also verified by several experiments [5] and numerical methods [1,6,7]. As a natural extension of spin ladders, one can imagine spin tubes, which mean spin ladders with the periodic boundary condition for the interchain (rung) direction. In contrast to spin ladders, the simple spin tubes as in Fig. 1(b) have

not been synthesized yet. However, quite recently, a few spin-tube-like materials [8,9] have been reported. It will accelerate the theoretical study of spin tubes. It is known that the above even-odd property of ladders breaks down in tubes: the odd-leg spin- $\frac{1}{2}$ tube with AF intrachain and rung couplings has doubly degenerate ground states with a spin gap [10].

Among these spin ladders and tubes, the 2-leg ladders have been studied most intensively. On the other hand, our understanding of ladders and tubes with higher chain numbers and spin magnitudes have not been progressed well, except for the above even-odd property. In this context, we consider the low-energy physics of simple spin ladders and tubes, models of Fig. 1, in this paper. Odd-leg AF-rung tubes have the frustration along the rung. For such frustrated tubes, the standard NLSM scheme, which assumes some short-range order to occur

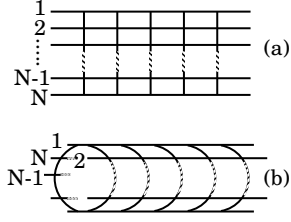


Fig. 1. N -leg spin ladder (a) and tube (b).

for the rung direction, is not applicable. In order to treat all systems containing frustrated tubes, we construct an alternative NLSM method, a simple extension of Sénéchal's method [11], which is a weak rung-coupling approach. As well known, a topological term appears in the NLSM for the half-integer-spin systems. Since it makes the analysis fairly complicated, we consider only integer-spin systems.

2. Model and method

The spin Hamiltonian, which we investigate, is

$$\mathcal{H} = J \sum_{n=1}^N \sum_j \mathbf{S}_{n,j} \cdot \mathbf{S}_{n,j+1} + J_{\perp} \sum_{n=1}^M \sum_j \mathbf{S}_{n,j} \cdot \mathbf{S}_{n+1,j} - h \sum_{n=1}^N \sum_j S_{n,j}^z, \quad (1)$$

where $\mathbf{S}_{n,j}$ is the integer-spin- s operator on site j of the n th chain, and $M = N - 1$ ($M = N$) for N -leg spin ladders (tubes: $\mathbf{S}_{N+1,j} = \mathbf{S}_{1,j}$). The intrachain coupling J is positive, i.e., AF. The final term represents the uniform Zeeman energy.

Let us explain the strategy dealing with the model (1) below. We start from the integer-spin- s AF chain: $H_n = J \sum_j \mathbf{S}_{n,j} \cdot \mathbf{S}_{n,j+1}$. Its low-energy physics can be described by an $O(3)$ NLSM. The partition function Z and Euclidean action A are

$$Z = \int D\mathbf{n} D\lambda \exp(-A[\mathbf{n}; \lambda]), \quad (2)$$

$$A = \int d\mathbf{x} \frac{-1}{2gc} \mathbf{n} \cdot (\partial_{\tau}^2 + c^2 \partial_x^2) \mathbf{n} - i\lambda(\mathbf{n}^2 - 1), \quad (3)$$

where $d\mathbf{x} = d\tau dx$ (τ : imaginary time, x : spatial coordinate), $\mathbf{n}(\mathbf{x})$ is a vector field with three compo-

nents, $g = 2/s$ is the coupling constant, $c = 2sJa_0$ (a_0 : lattice constant) is the spin-wave velocity, and $\lambda(\mathbf{x})$ is the Lagrange multiplier for the constraint $\mathbf{n}^2 = 1$. The spin operator is associated with the field \mathbf{n} through

$$\mathbf{S}_{n,j} \approx \frac{i}{4J} (\mathbf{n} \times \dot{\mathbf{n}}) + (-1)^j s \mathbf{n}, \quad (4)$$

where $\dot{\mathbf{n}} = \partial_{\tau} \mathbf{n}$. A simple estimation method of the lowest excitation energy of H_n , i.e., the Haldane gap, is the saddle-point approximation (SPA) for λ . It replaces the field λ with a constant λ_{sp} , which is determined by the saddle-point equation (SPE),

$$\partial A[\lambda_{sp}] / \partial \lambda_{sp} = 0, \quad (5)$$

where $A[\lambda]$ is defined as $e^{-A[\lambda]} = \int D\mathbf{n} e^{-A[\mathbf{n}; \lambda]}$. Employing the Fourier transformation, $\mathbf{n}(\mathbf{x}) \propto \sum_{\omega_n, k} e^{i(kx - \omega_n \tau)} \tilde{\mathbf{n}}(\omega_n, k)$, one can easily calculate $A[\lambda_{sp}]$, and then Eq. (5) becomes

$$\frac{3g}{2\pi} \ln \left[\Lambda \xi + \sqrt{1 + \Lambda^2 \xi^2} \right] = 1, \quad (6)$$

at zero temperature [12]. Here, Λ is the ultraviolet cut off of the wave number k , and $\xi^{-2} = -2ig\lambda_{sp}/c$. Through this SPA, the NLSM is mapped to a field theory of triply-degenerate bosons $n^{x,y,z}$ with the dispersion $\epsilon(k) = c\sqrt{k^2 + \xi^{-2}}$. These bosons may be interpreted as the lowest spin-1 magnons. Equation (6) determines the Haldane gap $\Delta(s) = c\xi^{-1}$ as

$$\Delta(s) = c\Lambda / \sinh(s\pi/3). \quad (7)$$

Since the accurate values of $\Delta(s)$ can be provided by numerical methods [13], Eq. (7) inversely fixes the cut off Λ . Therefore, NLSM plus SPA is a one-parameter-fitting theory [12].

We next take into account the rung-coupling term perturbatively. Namely, in the NLSM framework, we approximate it as

$$\sum_{n=1}^M \sum_j \mathbf{S}_{n,j} \cdot \mathbf{S}_{n+1,j} \rightarrow \frac{s^2}{a_0} \sum_{n=1}^M \int dx \mathbf{n}_n \cdot \mathbf{n}_{n+1}, \quad (8)$$

where the subscript n means the chain index. This prescription was first proposed by Sénéchal in the analysis of 2-leg ladders. It is clear that Eq. (8) is efficient even for frustrated tubes. From Eq. (8), it

is also found that the total action of the model (1) is a bilinear form of \mathbf{n}_n like the single-chain case. On the other hand, we have to treat N constraints, $\mathbf{n}_n^2 = 1$, differently from the single chain. Since the exact treatment of N constraints is considerably difficult, we replace them to an averaged one,

$$\sum_{n=1}^N \mathbf{n}_n^2 = N. \quad (9)$$

Relying on Eqs. (8) and (9), we study the model (1) in the following sections.

One should notice the following aspects. (i) The perturbative treatment (8) is valid only for the weak rung-coupling region. (ii) The averaging of constraints as in Eq. (9) would be a less accurate approximation for larger- N .

3. Cases without external fields

This section discusses the model (1) with $h = 0$. As mentioned already, the effective action of (1) is a bosonic bilinear form under the approximations (8) and (9). Therefore, even for ladders or tubes, we can utilize an SPA scheme in a similar way of the single-chain case. If we represent the Lagrange multiplier for Eq. (9) by the same symbol λ , its SPE becomes, at zero temperature,

$$\frac{3g}{2\pi} \sum_l \ln \left[\Lambda \xi_l + \sqrt{1 + \Lambda^2 \xi_l^2} \right] = N, \quad (10)$$

where $\xi_l^{-2} = \xi^{-2} + 2J_\perp \cos k_l / (Ja_0^2)$ and $k_l = \frac{\pi l}{N+1}$ ($l = 1, \dots, N$) [$k_l = \frac{2\pi l}{N}$ ($-\lceil \frac{N}{2} \rceil < l \leq \lceil \frac{N}{2} \rceil$)] for ladders [tubes]. (The symbol $[\alpha]$ stands for the maximum integer β satisfying $\beta \leq \alpha$.) In tubes, k_l means the wave number of the rung direction. Here, we used the same cut off Λ as that of the single chain. This SPA leads to $3N$ magnon bands with dispersions $\epsilon_l(k) = c\sqrt{k^2 + \xi_l^{-2}}$. The band splitting $\epsilon(k) \rightarrow \epsilon_l(k)$ is, of course, yielded from the hybridization among magnons due to the rung coupling. Each band $\epsilon_l(k)$ has a triple degeneracy, which corresponds to a spin-1 magnon triplet ($S^z = 1, 0$ and -1). Bands of *tubes* possesses *six-fold* degeneracy $\epsilon_l(k) = \epsilon_{-l}(k)$ except for $\epsilon_0(k)$ and

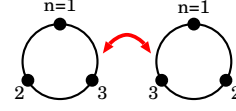


Fig. 2. Cross section and reflecting operation in 3-leg spin tube.

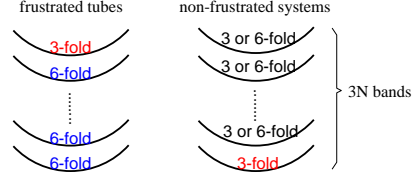


Fig. 3. Magnon band structures of N -leg systems. “ γ -fold” means the band has a γ -fold degeneracy. Six-fold degenerate bands do not appear in ladders.

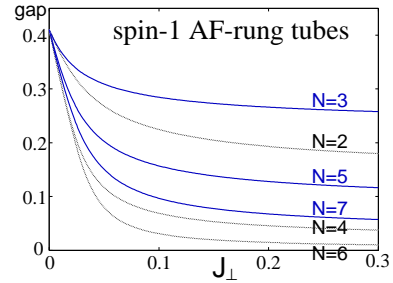


Fig. 4. Lowest excitation gaps in N -leg spin-1 AF-rung tubes with $J = 1$. In order to fix Λ in Eq. (10), we used the quantum Monte Carlo (QMC) data, $\Delta(1) = 0.410 \times J$ [13]. The “2-leg” tube means the 2-leg ladder.

$\epsilon_{N/2}(k)$. This extra degeneracy originates from the symmetry under the reflection about the plane including the central axis of tubes (see Fig. 2). Paying attention to these properties of $\epsilon_l(k)$, we can draw the magnon band structure as in Fig. 3. It is remarkable that *lowest bands of frustrated tubes have a six-fold degeneracy*, whereas all other systems have a standard triply degenerate lowest bands.

If we determine ξ from Eq. (10), we can discuss the band structure in more detail. Figure 4 represents the rung-coupling dependence of lowest excitation gaps in N -leg spin-1 AF-rung tubes. It shows that gaps decrease with increasing J_\perp and N , and gap reductions in frustrated (odd-leg) tubes are slower than those in non-frustrated tubes. The latter must reflect the fact that the growth of the AF short-range order is disturbed in frustrated tubes. Although all gaps monotonically decrease with in-

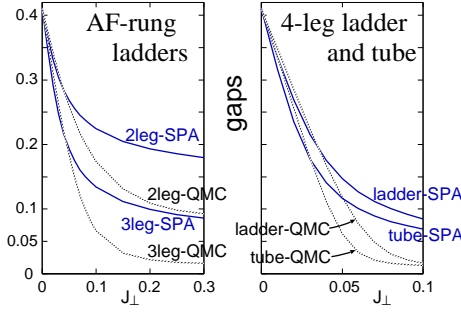


Fig. 5. Gaps of SPA and QMC methods in spin-1 AF-rung ladders or tubes with $J = 1$. The QMC data is provided by Munehisa Matsumoto.

creasing J_{\perp} within the present scheme, one should recall that the scheme is valid especially for the weak rung-coupling region. Actually, it is known and easily expected that the gap growth of the 2-leg spin-1 AF-rung ladder turns from a decrease to an increase as J_{\perp} exceeds $O(J)$ [14].

Finally, let us compare our results with the ones of the QMC method. From Fig. 5, it is expected that our results are semi-quantitatively correct within $|J_{\perp}| < 0.05 \times J$, and are qualitatively reliable even for the weak rung-coupling case of $|J_{\perp}| > 0.05 \times J$. The main origin of the deviation between two data would lie in approximations (8) and (9), and the SPA.

4. External-field effects

We consider the effect of the uniform Zeeman term briefly. To do so, we should note the following general features. (i) All excitations with $\epsilon_l(k)$ are regarded as spin-1 magnons. (ii) The uniform field h in Eq. (1) induces the Zeeman splitting of spin-1 magnons, and the magnon band with $S^z = +1$ goes down linearly with h . (iii) In general, when a magnon condensation occurs in a 1D spin system conserving the z component of the total spin, the ground state becomes one-component Tomonaga-Luttinger liquid (TLL) [15,16].

Taking into account (i)-(iii) and the band structure in the previous section, one can expect that a sufficiently strong field h induces a two (one)-component TLL for frustrated tubes (non-frustrated ladders and tubes).

5. Summary

We investigated low-lying magnon excitations of integer-spin ladders and tubes (1) in the weak rung-coupling region. It was found that lowest excitations of frustrated tubes consist of six-fold degenerate magnon bands, while those of all other systems are standard triply degenerate ones. In addition, we can also expect that a two (one)-component TLL emerges in frustrated tubes (non-frustrated systems), as the field h increases enough. This expectation, however, is based on the analysis, in which the field h does not reach the lower critical value. We will revisit the effects of the Zeeman term via other approaches [15,16,17], elsewhere. Furthermore, we will discuss more detail of our method here and effects of other external fields elsewhere.

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